Lefschetz thimble approach to the fermion sign problem

Yuya Tanizaki

RIKEN BNL Research Center, Brookhaven National Laboratory

Sep 20, 2017 @ Keio University

Collaborators: Takayuki Koike (Kyoto), Takuya Kanazawa (RIKEN), Hiromichi Nishimura (RIKEN BNL), Kouji Kashiwa (Kyoto), Kenji Fukushima (Tokyo), Yoshimasa Hidaka (RIKEN), Tomoya Hayata (Chuō), Motoi Tachibana (Saga)

Contents

Motivation: Monte Carlo simulation and Sign problem

Method: Path integral on Lefschetz thimbles

Applications: Case studies of fermionic sign problem

Motivation: Monte Carlo simulation and Sign problem

Path integral and Monte Carlo simulation

To characterize the thermal state, we can use path integral,

$$Z = \mathrm{tr}_{\mathcal{H}}\left[\mathrm{e}^{-\beta \hat{H}}\right] = \int_M \mathcal{D}A \exp(-S[A]).$$

The integration domain M (of an $SU(N)$ gauge theory) is

$$M = SU(N)^{\beta\cdot\mathrm{Volume}}.$$

We want a tool to evaluate Z without exponential complexity.

Monte Carlo method: Consider the case $\mathrm{e}^{-S[A]} \geq 0$.
Generate an ensemble $\{A_i\}_i$ following $\frac{1}{Z}\mathrm{e}^{-S[A]}$, and evaluate

$$\langle O(A)\rangle \simeq \frac{1}{N}\sum_{i=1}^{N} O(A_i).$$

More about Monte Carlo simulation

Do we really circumvent exponential complexity using MC method?

$$\text{Error of } \frac{1}{N}\sum_{i=1}^{N} O(A_i) = \frac{\text{Typical values of } |O(A_i) - \langle O\rangle|}{\sqrt{N}}.$$

It indeed solves the exponential complexity for operators satisfying

$$\frac{\langle O(A)\rangle}{\text{Typical values of } |O(A_i) - \langle O\rangle|} \sim (\beta \cdot \mathrm{Volume})^{-\#}.$$

It has been quite successful to understand Hadron structures, thermodynamics of finite-temperature QCD, etc.

This argument is true only when $\mathrm{e}^{-S[A]} \geq 0$.

Sign problem and Exponential complexity

To use Monte Carlo method when $\mathrm{e}^{-S[A]} \not\geq 0$, we generate the ensemble $\{A_i\}_i$ following the phase-quenched distribution $\mathrm{e}^{-\mathrm{Re}(S[A])}$:

$$\langle O(A)\rangle = \frac{\langle O(A)\mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}\rangle_{\mathrm{p.q.}}}{\langle \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}\rangle_{\mathrm{p.q.}}} \simeq \frac{\frac{1}{N}\sum_{i=1}^{N} O(A_i)\mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}}{\frac{1}{N}\sum_{i=1}^{N} \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}}.$$

Since $\langle \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}\rangle_{\mathrm{p.q.}} = \mathrm{e}^{-\beta\cdot\mathrm{Volume}\,\Delta f}$. Thus,

$$\text{Necessary } N \text{ of configurations} \gtrsim \mathrm{e}^{2\beta\cdot\mathrm{Volume}\,\Delta f}.$$

Exponential complexity revives due to the sign problem.

Question

Can we make $\Delta f = 0$ by inventing a clever technique?

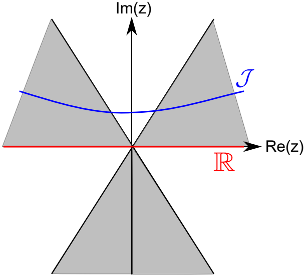
Method: Path integral on Lefschetz thimbles

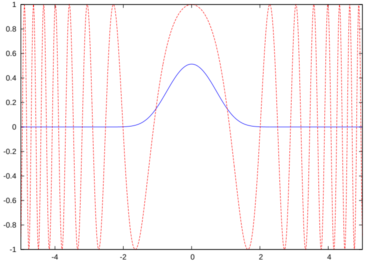
Lefschetz thimble for Airy integral

Airy integral is given as

$$\mathrm{Ai}(a) = \int_{\mathbb{R}} \frac{\mathrm{d}x}{2\pi} \exp \mathrm{i} \left(\frac{x^3}{3} + ax \right)$$

Complexify the integration variable: $z = x + \mathrm{i}y$.





Integrand on $\mathbb{R}$, and on $\mathcal{J}_1$ $(a = 1)$

Multiple integrals on Lefschetz thimbles

Oscillatory integrals with **many variables** can be evaluated using the "steepest descent" cycles $\mathcal{J}_\sigma$: (classical eom $S'(z_\sigma)=0$)

$$\int_M \mathrm{d}^n x\, \mathrm{e}^{-S(x)} = \sum_\sigma \langle \mathcal{K}_\sigma, M\rangle \int_{\mathcal{J}_\sigma} \mathrm{d}^n z\, \mathrm{e}^{-S(z)}.$$

Unlike one-dimensional case, the steepest descent manifold is not uniquely defined.

$\Rightarrow$ Use of the homology $H_n(M_\mathbb{C}, \{\mathrm{e}^{-\mathrm{Re}(S)} \ll 1\})$ becomes quite essential:

$$\begin{aligned} H_n(M_\mathbb{C}, \{\mathrm{e}^{-\mathrm{Re}(S)} \ll 1\}) &\simeq \sum_\sigma \mathbb{Z}[\mathcal{J}_\sigma], \\ H_n(M_\mathbb{C} \setminus \{\mathrm{e}^{-\mathrm{Re}(S)} \ll 1\}) &\simeq \sum_\sigma \mathbb{Z}[\mathcal{K}_\sigma]. \end{aligned}$$

[Pham, 1967; Kaminski, 1994; Howls, 1997]

Multiple integrals on Lefschetz thimbles

Concrete construction Pick up a metric $\mathrm{d}s^2 = g_{i\bar{j}}\mathrm{d}z^i \otimes \mathrm{d}\overline{z^j}$, and consider the gradient flow:

$$\frac{\mathrm{d}z^i(t)}{\mathrm{d}t} = g^{i\bar{j}}\overline{\left(\frac{\partial S(z)}{\partial z^j}\right)}.$$

$\mathcal{J}_\sigma$ are called Lefschetz thimbles, and $\mathrm{Im}[S]$ is constant on it:

$$\mathcal{J}_\sigma = \left\{ z(0) \middle| \lim_{t\to-\infty} z(t) = z_\sigma \right\}.$$

Similarly, $\mathcal{K}_\sigma = \{z(0)|z(\infty) = z_\sigma\}$.

[Pham, 1967; Kaminski, 1994; Howls, 1997, Witten, arXiv:1001.2933, 1009.6032]

[Christoforetti et al. (PRD(2012)), Fujii et al. (JHEP 1310), etc.]

Monte Carlo algorithm on Lefschetz thimbles

Monte Carlo algorithms on thimble(s) has been developing:

- Langevin on $\mathcal{J}_\sigma$ Cristoforetti, Di Renzo, Scorzato, 1205.3996
- Hybrid MC on $\mathcal{J}_\sigma$ Fujii, Honda, Kato, Kikukawa, Komatsu, Sano, 1309.4371
- Contraction algorithm Alexandru, Basar, Bedaque, 1510.03258
- Generalized thimble Alexandru, Basar, Bedaque, Ridgway, Warrington, 1512.08764

These methods generate ensembles $\{z_i\}_i$ on $\mathcal{J}_\sigma$ following $\mathrm{e}^{-S(z)}$:

$$\frac{1}{Z}\int_{\mathcal{J}_\sigma} \mathrm{d}^n z O(z) \exp(-\hbar^{-1}S(z)) \simeq \frac{\frac{1}{N}\sum_{i=1}^{N}\frac{\mathrm{d}^n z_i}{|\mathrm{d}^n z_i|}O(z_i)}{\frac{1}{N}\sum_{i=1}^{N}\frac{\mathrm{d}^n z_i}{|\mathrm{d}^n z_i|}}.$$

N.B. $\int_{\mathcal{J}_\sigma}$ satisfies resurgence for "nice" S (Berry, Howls, '91, Howls '97).

"Reweighting factor" for Lefschetz thimble

We define the "reweighting factor" of the Lefschetz-thimble approach by

$$\exp(-\beta \cdot \mathrm{Volume}\,\Delta f) \equiv \frac{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \mathrm{d}z \exp(-S(z))}{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} |\mathrm{d}z| \exp(-\mathrm{Re}(S(z)))}.$$

cf. Reweighting factor in the conventional approach:

$$\exp(-\beta \cdot \mathrm{Volume}\,\Delta f) \equiv \frac{\int_M \mathrm{d}x \exp(-S(x))}{\int_M \mathrm{d}x \exp(-\mathrm{Re}(S(x)))}.$$

Idea of this talk: Comparison of these Δf tells us the property of the Lefschetz-thimble approach.

Applications: Case studies of fermionic sign problem

- One-site Hubbard model (1509.07146, with Tomoya Hayata, Yoshimasa Hidaka)
- Multi-flavor massless QED_2 (1612.06529, with Motoi Tachibana)

Case 1 One-site Hubbard model

Path integral for one-site Hubbard model

We consider the $(0+1)$-dimensional fermion model,

$$S=\int_0^\beta \mathrm{d}\tau\left(\frac{\phi(\tau)^2}{2U}+\psi^*[\partial_\tau+(-U/2-\mu-\mathrm{i}\phi(\tau))]\psi\right).$$

The path-integral expression for the one-site Hubbard model $(\varphi=\frac{1}{\beta}\int_0^\beta \mathrm{d}\tau\phi(\tau))$:

$$Z=\sqrt{\frac{\beta}{2\pi U}}\int_{\mathbb{R}}\mathrm{d}\varphi\underbrace{\left(1+\mathrm{e}^{\beta(\mathrm{i}\varphi+\mu+U/2)}\right)^2}_{\text{Fermion Det}}\mathrm{e}^{-\beta\varphi^2/2U}.$$

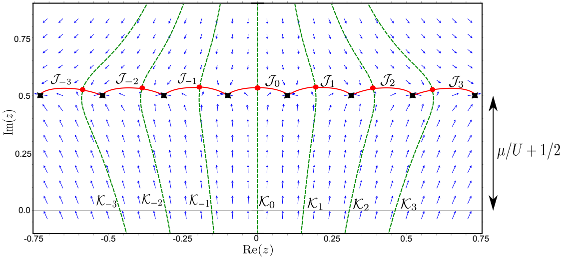
Integrand has complex phases causing the sign problem.

φ is an auxiliary field for the fermion number density:

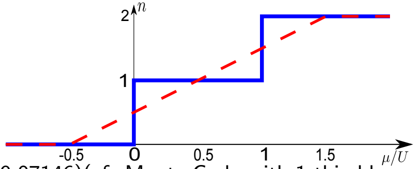
$$\langle\hat{n}\rangle=\mathrm{Im}\langle\varphi\rangle/U.$$

Behaviors of number density and Lefschetz thimbles

Lefschetz thimbles with $-0.5U < \mu < 1.5\mu$:



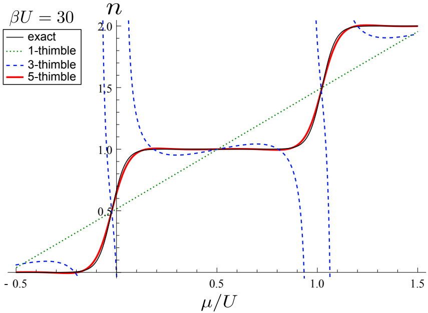
Number density n with exact result and one-thimble result:

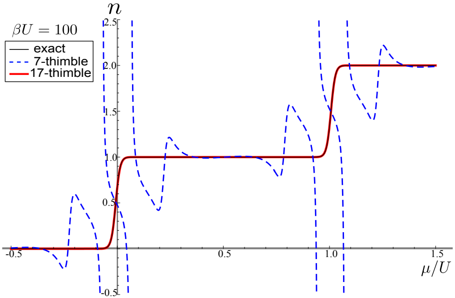


(YT, Hidaka, Hayata, 1509.07146)(cf. Monte Carlo with 1-thimble approx. gives a wrong result: Fujii, Kamata, Kikukawa,1509.08176, 1509.09141; Alexandru, Basar, Bedaque,1510.03258.)

Results

Results for $\beta U = 30, 100$: (YT, Hidaka, Hayata, 1509.07146)





Necessary numbers of Lefschetz thimbles $\simeq \beta U/2\pi$.

(cf. Fujii, Kamata, Kikukawa,1509.08176, 1509.09141; Alexandru, Basar, Bedaque,1510.03258)

Consequence

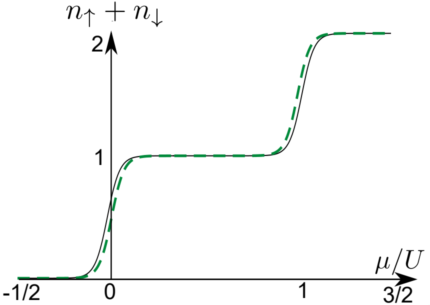
In order to describe the step functions, we need interference of complex phases among different Lefschetz thimbles.

Semiclassical partition function

Using complex classical solutions z_m, let us calculate the semiclassical partition function (YT, Hidaka, Hayata, 1509.07146):

$$Z_{\rm cl} := \sum_{m=-\infty}^{\infty} \mathrm{e}^{-S_m} = \mathrm{e}^{-S_0(\mu)} \theta_3 \left(\pi \left(\frac{\mu}{U} + \frac{1}{2} \right), \mathrm{e}^{-2\pi^2/\beta U} \right).$$

This expression is a good approximation for $-1/2 \lesssim \mu/U \lesssim 3/2$.



Sign problem after Lefschetz-thimble deformation

This computation means that the sign problem exists after the Lefschetz-thimble deformation.
Compute the reweighting factor:

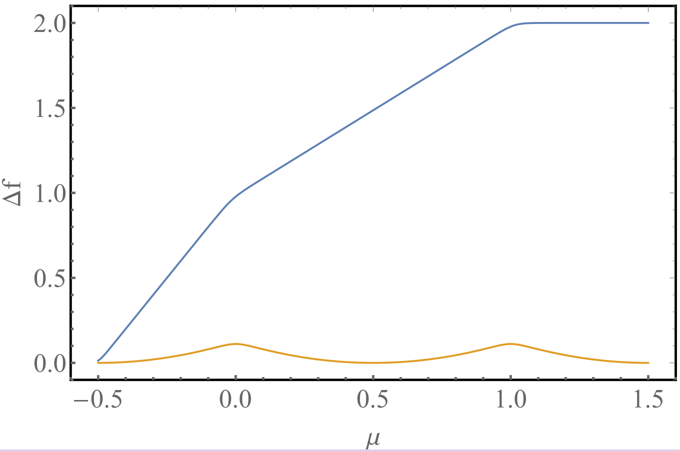
$$\frac{\int_{\sum_m \mathcal{J}_m} \mathrm{d}z \mathrm{e}^{-S(z)}}{\int_{\sum_m \mathcal{J}_m} |\mathrm{d}z| \mathrm{e}^{-\mathrm{Re}(S(z))}} \simeq \frac{\sum_m \mathrm{e}^{-S_m}}{\sum_m \mathrm{e}^{-\mathrm{Re}(S_m)}} = \frac{\theta_3\left(\pi\left(\frac{\mu}{U}+\frac{1}{2}\right), \mathrm{e}^{-2\pi^2/\beta U}\right)}{\theta_3\left(0, \mathrm{e}^{-2\pi^2/\beta U}\right)}.$$

At $\mu = 0$, for example,

$$\frac{\int_{\sum_m \mathcal{J}_m} \mathrm{d}z \mathrm{e}^{-S(z)}}{\int_{\sum_m \mathcal{J}_m} |\mathrm{d}z| \mathrm{e}^{-\mathrm{Re}(S(z))}} \simeq \exp\left(-\beta \frac{U}{8}\right).$$

We find nonzero Δf.

Comparison between naive reweighting and thimbles



Consequence

Lefschetz-thimble method reduces Δf in the one-site Hubbard model, but it is still nonzero.

Case 2 Massless QED_2

Multi-flavor massless QED$_2$

2-dimensional $U(1)$ gauge theories with N_f massless fermions:

$$Z = \int \mathcal{D}A\, \mathrm{e}^{-S_{\mathrm{ph}}[A]} \int \mathcal{D}\overline{\psi}\mathcal{D}\psi \exp\left(-\sum_{a=1}^{N_f} \int \mathrm{d}^2 x\, \overline{\psi}_a \left[D_A - \mu_a \gamma^0\right] \psi_a\right)$$

Since the fermions are massless, the nonzero topological sectors do not appear:

$$A = \underbrace{\frac{2\pi}{\beta} h_0 \mathrm{d}x^0 + \frac{2\pi}{L} h_1 \mathrm{d}x^1}_{\text{toron}} + \underbrace{*\mathrm{d}\phi}_{\text{photon}} + \underbrace{\mathrm{d}\lambda}_{\text{gauge}} .$$

ϕ-dependence is computable using the anomaly equation, and does not have the sign problem.

Toron-field integral of multi-flavor massless QED$_2$

The toron-field integration becomes ($\tau = L/\beta$: temperature)

$$Z = \int_0^1 \mathrm{d}h_0 \mathrm{d}h_1 \exp\left[-\frac{2\pi}{\tau} F(h_0, h_1)\right],$$

where F is the fermion one-loop free energy ($\mu'_a = L\mu_a/(2\pi)$),

$$F = N_f \left(h_1 - \frac{1}{2}\right)^2 - \frac{\tau}{2\pi} \sum_{a=1}^{N_f} \sum_{n=1}^{\infty} \Big\{ \ln\left(1 + \mathrm{e}^{-\frac{2\pi}{\tau}(n+h_1-1-\mu'_a)-2\pi\mathrm{i}h_0}\right) + \ln\left(1 + \mathrm{e}^{-\frac{2\pi}{\tau}(n-h_1+\mu'_a)+2\pi\mathrm{i}h_0}\right) + \ln\left(1 + \mathrm{e}^{-\frac{2\pi}{\tau}(n+h_1-1+\mu'_a)+2\pi\mathrm{i}h_0}\right) + \ln\left(1 + \mathrm{e}^{-\frac{2\pi}{\tau}(n-h_1-\mu'_a)-2\pi\mathrm{i}h_0}\right) \Big\}.$$

In the limit $\tau \to 0$, we can use the mean-field approximation with complex saddle points (1612.06529, with Motoi Tachibana) (cf.1504.02979, with Hiromichi Nishimura, Kouji Kashiwa).

Gradient flow for massless QED$_2$

All the relevant complex saddle points have real F:

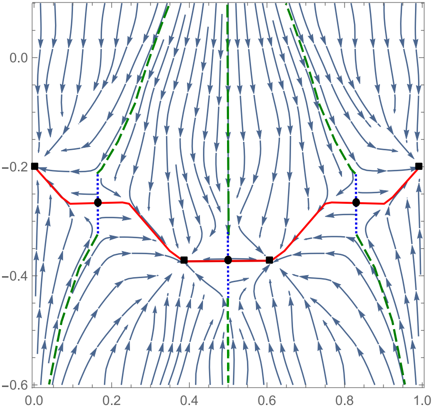
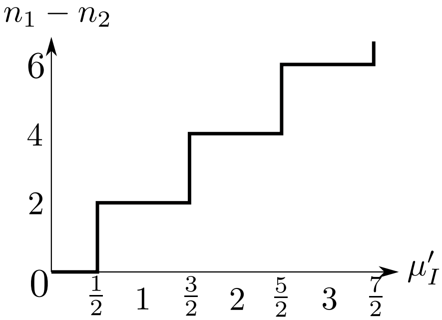


Figure: Gradient flow in the $\mathrm{Re}(h_1)$-$\tau\mathrm{Im}(h_0)$ plane at $N_f = 3$

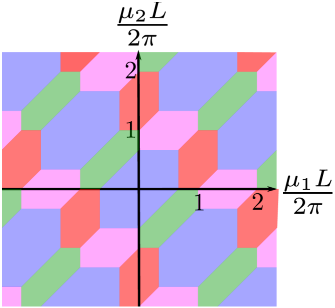
(1612.06529, with Motoi Tachibana)

Phase structure of multi-flavor massless QED$_2$

At the zero-temperature with finite L, $\tau = 0$, the first-order transition occurs in this model:



(a) Fermion number at $N_f = 2$



(b) Phase boundary at $N_f = 3$

(1612.06529, with Motoi Tachibana) (The results are consistent with the exact computation given by Lohmayer, Narayanan, 1307.4969)

Sign problem after Lefschetz-thimble deformation

In the N_f-flavor massless QED_2, there are only N_f relevant saddle points in the limit $\tau \to 0$.

Since the (complex) mean-field approx. is good in this limit after the Lefschetz-thimble deformation, one can show that

$$\frac{\int_{\sum_m \mathcal{J}_m} \mathrm{d}^2 h\, \mathrm{e}^{-S(h)}}{\int_{\sum_m \mathcal{J}_m} |\mathrm{d}^2 h| \mathrm{e}^{-\mathrm{Re}(S(h))}} \simeq 1$$

This implies that $\Delta f = 0$ (at least in the limit $\tau \to 0$).

Consequence

Lefschetz-thimble method solves the sign problem of massless QED_2.

Summary

- The sign problem is reviewed from the viewpoint of exponential complexity.
- Using Cauchy's theorem, one can deform the oscillatory integral into the sum of steepest descent integrals on Lefschetz thimbles
- We consider two examples of the fermionic sign problem.
  In the one-site model, the exponential complexity is not solved, but Δf is reduced.
  In massless QED_2, the exponential complexity is eliminated by using Lefschetz thimbles.